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The number of independent sets in unicyclic graphs with a given diameter☆

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ABSTRACT

Let $\mathcal{U}_{n,d}$ denote the set of unicyclic graphs with a given diameter d. In this paper, the unique unicyclic graph in $\mathcal{U}_{n,d}$ with the maximum number of independent sets, is characterized.

1. Introduction

Let G be a graph on n vertices. Two vertices of G are said to be *independent* if they are not adjacent in G. An *independent* k-set is a set of k vertices, no two of which are adjacent. Denote by $\sigma(G, k)$ the number of the k-independent sets of G. It follows directly from the definition that $\emptyset$ is an independent set. Then $\sigma(G, 0) = 1$ for any graph G. The total number of independent sets of G, denoted by $\sigma(G)$, is defined as

$$\sigma(G) = \sum_{k=0}^{n} \sigma(G, k).$$

The first papers about counting maximum independent sets in a graph are those of Miller and Muller [19] and Moon and Moser [20]. For a survey see [4,5].

In chemical literature the graph parameter $\sigma(G)$ is denoted by $i(G)$, and it is referred to as the *Merrifield–Simmons index*. It is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [18]. There, Merrifield and Simmons showed the correlation between this index and boiling points. After that some results on this topological index appeared (e.g., see, [3,8–11]).

The total number of independent sets of a graph G is also called the *Fibonacci number* of the graph G. It was introduced in 1982 in a paper of Prodinger and Tichy [22]. Recently, there have been many papers studying the Fibonacci number of a graph. In [1], Alameddine studied bounds for the Fibonacci number of a maximum outer planar graph. Gutman [12], Zhang and Tian [27,28] studied the Fibonacci number for hexagonal chains and catacondensed systems, respectively. In [13], Li et al., characterized the tree with the maximum Fibonacci number among the trees with a given diameter. In [14], Zhao and Li investigated the orderings of two classes of trees by their Fibonacci numbers, and used these orderings to determine

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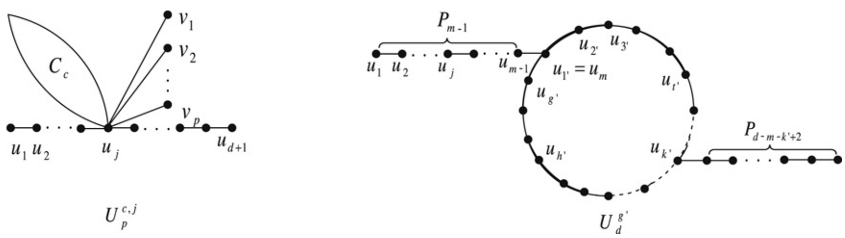

Fig. 1. Graphs $U_p^{c,j}$ and $U_d^{g'}$.

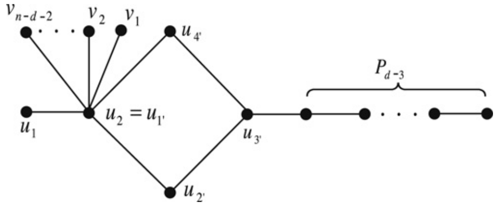

Fig. 2. Graph $\bar{U}^{4,2}_{n-d-2}$.

the unique tree with the second (and respectively the third) smallest Fibonacci number among all trees with n vertices. In [21], Pedersen and Vestergaard studied the Fibonacci number for the unicyclic graphs. In [25], Yu and Tian studied the Fibonacci numbers of the graphs with given edge-independence number and cyclomatic number. Yu and Lv [17,26] studied the Fibonacci numbers of trees with maximum degree and given pendent vertices, respectively. Ye et al., ordered the unicyclic graphs with given girth according to the Fibonacci numbers in [24].

The problem of counting the number of independent sets in a graph is NP-complete (see for instance Roth [23]). When dealing with a graph parameter for which the value is NP-complete to determine, it is often useful to find bounds for its values. Chou and Chang [6] gave an upper bound on the number of maximum independent sets in graphs with, at most, one cycle. In 2005, Pedersent and Vestergaard gave upper and lower bounds for the total number of independent sets in unicyclic graphs [21]. In this paper, we consider the total number of independent sets in unicyclic graphs with given diameter d. In particular, we prove that every unicyclic graph G on n vertices with diameter d satisfies $\sigma(G) \leqslant 2^{n-d-1}(2F_{d-2} + F_d) + F_{d-1}$ for $d \geqslant 4$, while for $d = 3$, $\sigma(G) \leqslant 5 \cdot 2^{n-4} + 2$ and we characterize the extremal graphs for these inequalities, where F_n is the n-th Fibonacci number, defined by $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = F_1 = 1$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bondy and Murty [2]. We only consider finite, undirected and simple graphs. For a vertex v of a graph G, we denote $N(v) = \{u|uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$. A *pendent vertex* is a vertex of degree 1. For two vertices x and y ($x \neq y$), the *distance* between x and y is the number of edges in a shortest path joining x and y. The *diameter* of a graph G is the maximum distance between any two vertices of G. A *unicyclic graph* is a connected graph with n vertices and n edges, we shall by $\mathcal{U}_{n,d}$ denote the set of all unicyclic graphs on n vertices with diameter d.

If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. We denote by P_n, C_n and $K_{1,n-1}$ the path, the cycle and the star on n vertices, respectively. We use $VL(G)$ to denote the vertex set $\{v : v \in V(G) \text{ and } d(v) = 1\}$.

In order to formulate our results, some unicyclic graphs need to be defined, as follows. Let $U_p^{c,j}$ denote a unicyclic graph on n vertices with diameter d created from a path $P_{d+1} = u_1u_2 \ldots u_j \ldots u_{d+1}$ by attaching a cycle C_c and p pendent vertices $v_1, v_2, \ldots, v_p$ to u_j on P_{d+1} such that $c + p + d = n$ (see Fig. 1).

Let $U_d^{g'}$ denote the unicyclic graph with diameter d created from a cycle $C_{g'} = u_{1'}u_{2'} \cdots u_{t'} \cdots u_{k'} \cdots u_{h'} \cdots u_{g'}u_{1'}$ by joining a vertex $u_{1'}$ (respectively, $u_{k'}$) of $C_{g'}$ to an end vertex of P_{m-1} (respectively, $P_{d-m-k'+2}$), where $1 \leqslant k' \leqslant \frac{1}{2}g'$ (see Fig. 1).

Let $\bar{U}^{g',i}_{n-d-g'+k-1,m}$ be a unicyclic graph on n vertices with diameter d created from $U_d^{g'}$ by attaching $n - d - g' + k' - 1$ pendent vertices $v_1, v_2, \ldots, v_{n-d-g'+k'-1}$ to a non-pendent vertex u_i in $V(U_d^{g'})$.

In this paper, we show that $\bar{U}^{4,2}_{n-d-2,2}$ (e.g., see Fig. 2) is the unique graph in $\mathcal{U}_{n,d}$ with the maximum Fibonacci number.

We list some lemmas that will be used in this paper.

Lemma 1.1 ([7]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $\sigma(G) = \sigma(G - uv) - \sigma(G - (N[u] \cup N[v]))$;*
(ii) *If $v \in V(G)$, then $\sigma(G) = \sigma(G - v) + \sigma(G - N[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $\sigma(G) = \prod_{j=1}^{t} \sigma(G_j)$.*

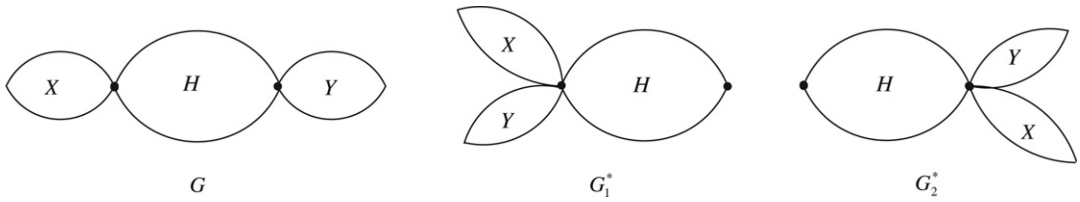

Fig. 3. Graphs G, G_1^* and G_2^*.

Lemma 1.2 ([14]). *Let $n = 4s + r$, where n, s and r are integers with $0 \le r \le 3$.*

(i) *If $r \in \{0, 1\}$, then*

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} \\ &> F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1}; \end{aligned}$$

(ii) *If $r \in \{2, 3\}$, then*

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} \\ &> F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}. \end{aligned}$$

Two graphs are said to be *disjoint* if they have no vertex in common.

Lemma 1.3 ([15]). *Let H, X, Y be three connected graphs disjoint in pairs. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'; see Fig. 3. Then*

$$\sigma(G_1^*) > \sigma(G) \quad \text{or} \quad \sigma(G_2^*) > \sigma(G).$$

Let H_1, H_2 be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let $G = H_1vH_2$ be a graph defined by $V(G) = V(H_1) \cup V(H_2)$ and $E(G) = E(H_1) \cup E(H_2)$.

Lemma 1.4 ([16]). *Let H be a connected graph and T_l be a tree of order $l+1$ with $V(H) \cap T_l = \{v\}$. Then $\sigma(HvT_l) \leqslant \sigma(HvK_{1,l})$, the equality holds if, and only if, $HvT_l \cong HvK_{1,l}$, where v is identified with the center of the star $K_{1,l}$ in $HvK_{1,l}$.*

2. Lemmas and main results

According to the definitions of the Fibonacci number of a graph, by Lemma 1.1, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$. In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $\sigma(G) = \sigma(G - v) + \sigma(G - \{u, v\})$. So it is easy to see that $\sigma(P_0) = 1, \sigma(P_1) = 2$ and $\sigma(P_n) = \sigma(P_{n-1}) + \sigma(P_{n-2})$ for $n \geqslant 2$. Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. We have

$$\sigma(P_n) = F_{n+1} = \frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+2} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+2}\right].$$

Note that $F_{n+m} = F_nF_m + F_{n-1}F_{m-1}$. For convenience, we let $F_n = 0$, if $n < 0$. By Lemma 1.1, we obtain the following results.

Lemma 2.1. *For graph $U_{n-d-g'+k'-1}^{g'-k'+1,j}$, we have*

$$\sigma(U_{n-d-g'+k'-1}^{g'-k'+1,j}) = 2^{n-d-g'+k'-1}F_jF_{d+2-j}F_{g'-k'+1} + F_{j-1}F_{d+1-j}F_{g'-k'-1}.$$

Proof. By Lemma 1.1,

$$\begin{aligned} \sigma(U_p^{c,j}) &= \sigma(U_p^{c,j} - u_j) + \sigma(U_p^{c,j} - N[u_j]) \\ &= \sigma(P_{j-1} \cup P_{c-1} \cup P_{d+1-j} \cup \{v_1, \ldots, v_p\}) + \sigma(P_{j-2} \cup P_{c-3} \cup P_{d-j}) \\ &= 2^pF_jF_cF_{d+2-j} + F_{j-1}F_{c-2}F_{d+1-j}. \end{aligned}$$

Taking $p = n - d - g' + k' - 1$ and $c = g' - k' + 1$ gives the result. □

Lemma 2.2. *In $U_d^{g'}$, set $P_x := u_{1'}u_{g'}\cdots u_{h'}$, $P_y := u_{h'}u_{h'-1}\cdots u_{k'+1}u_{k'}$, $P_{x'} := u_{1'}u_{2'}\cdots u_{t'}$, $P_{y'} := u_{t'}u_{t'+1}\cdots u_{k'-1}u_{k'}$ and $P_l := P_{d-m-k'+2}$. Let $k' < h' \le g'$ and $1 < t' < k'$. Then*

$$\begin{aligned}
&\text{(i) } \sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m}) = 2^{n-d-g'+k'-1}F_{l+1}(F_mF_{k'-1}F_{g'-k'+1} + F_{m-1}F_{k'-2}F_{g'-k'})\\
&\qquad + F_lF_mF_{k'-2}F_{g'-k'} + F_lF_{m-1}F_{k'-3}F_{g'-k'-1}.\\
&\text{(ii) } \sigma(\bar{U}^{g',h'}_{n+k'-d-g'-1,m}) = (2^{n-d-g'+k'-1}-1)(F_mF_{x-1}F_{y-1}F_{l+1}F_{k'-1} + F_mF_{x-1}F_{y-2}F_lF_{k'-2}\\
&\qquad + F_{m-1}F_{x-2}F_{y-1}F_{l+1}F_{k'-2} + F_{m-1}F_{x-2}F_{y-2}F_lF_{k'-3}) + F_mF_{g'-k'+1}F_{l+1}F_{k'-1} + F_mF_{g'-k'}F_lF_{k'-2}\\
&\qquad + F_{m-1}F_{g'-k'}F_{l+1}F_{k'-2} + F_{m-1}F_{g'-k'-1}F_lF_{k'-3}.\\
&\text{(iii) } \sigma(\bar{U}^{g',t'}_{n+k'-d-g'-1,m}) = (2^{n-d-g'+k'-1}-1)(F_mF_{x'-1}F_{y'-1}F_{l+1}F_{g'-k'+1} + F_mF_{x'-1}F_{y'-2}F_lF_{g'-k'}\\
&\qquad + F_{m-1}F_{x'-2}F_{y'-1}F_{l+1}F_{g'-k'} + F_{m-1}F_{x'-2}F_{y'-2}F_lF_{g'-k'-1})\\
&\qquad + F_mF_{k'-1}F_{l+1}F_{g'-k'+1} + F_mF_{k'-2}F_lF_{g'-k'} + F_{m-1}F_{k'-2}F_{l+1}F_{g'-k'} + F_{m-1}F_{k'-3}F_lF_{g'-k'-1}.\\
&\text{(iv) } \sigma(\bar{U}^{g',j}_{n+k'-d-g'-1,m}) = 2^{n-d-g'+k'-1}(F_jF_{m-j}F_{g'-k'+1}F_{l+1}F_{k'-1} + F_jF_{m-j}F_{g'-k'}F_lF_{k'-2}\\
&\qquad + F_jF_{m-j-1}F_{g'-k'}F_{l+1}F_{k'-2} + F_jF_{m-j-1}F_{g'-k'-1}F_lF_{k'-3})\\
&\qquad + F_{j-1}F_{m-j-1}F_{g'-k'+1}F_{l+1}F_{k'-1} + F_{j-1}F_{m-j-1}F_{g'-k'}F_lF_{k'-2}\\
&\qquad + F_{j-1}F_{m-j-2}F_{g'-k'}F_{l+1}F_{k'-2} + F_{j-1}F_{m-j-2}F_{g'-k'-1}F_lF_{k'-3}.
\end{aligned}$$

Proof. (i) Let $T = \bar{U}^{g',k'}_{n+k'-d-g'-1,m} - P_l - \{v_k, v_1, v_2, \ldots, v_{n-d-g'+k'-1}\}$, $T' = T - \{v_{k'-1}, v_{k'+1}\}$. Applying Lemma 1.1(ii) just one time to $u_{k'}$, Eq. (2.1) holds immediately.

$$\sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m}) = 2^{n-d-g'+k'-1}F_{l+1}\sigma(T) + F_l\sigma(T'). \tag{2.1}$$

Furthermore,

$$\begin{aligned}
\sigma(T) &= \sigma(T-u_{1'}) + \sigma(T-N[u_{1'}])\\
&= \sigma(P_{m-1}\cup P_{k'-2}\cup P_{g'-k'}) + \sigma(P_{m-2}\cup P_{k'-3}\cup P_{g'-k'-1})\\
&= F_mF_{k'-1}F_{g'-k'+1} + F_{m-1}F_{k'-2}F_{g'-k'},
\end{aligned} \tag{2.2}$$

$$\begin{aligned}
\sigma(T') &= \sigma(T'-u_{1'}) + \sigma(T'-N[u_{1'}])\\
&= \sigma(P_{m-1}\cup P_{k'-3}\cup P_{g'-k'-1}) + \sigma(P_{m-2}\cup P_{k'-4}\cup P_{g'-k'-2})\\
&= F_mF_{k'-2}F_{g'-k'} + F_{m-1}F_{k'-3}F_{g'-k'-1}.
\end{aligned} \tag{2.3}$$

By (2.1)–(2.3), we have

$$\sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m}) = 2^{n-d-g'+k'-1}F_{l+1}(F_mF_{k'-1}F_{g'-k'+1} + F_{m-1}F_{k'-2}F_{g'-k'}) + F_lF_mF_{k'-2}F_{g'-k'} + F_lF_{m-1}F_{k'-3}F_{g'-k'-1}.$$

(ii) Let

$$\begin{aligned}
&T_1 = \bar{U}^{g',h'}_{n+k-d-g'-1,m} - \{u_{h'}, v_1, v_2, \ldots, v_{n-d-g+k-1}\}, \qquad T_1' = T_1 - \{u_{h'-1}, u_{h'+1}\},\\
&T_2 = T_1 - (P_{m-1}\cup P_x), \qquad T_2' = T_2 - u_{2'}.
\end{aligned}$$

Applying Lemma 1.1(ii) to $u_{h'}$, Eq. (2.4) holds immediately.

$$\sigma(\bar{U}^{g',h'}_{n+k'-d-g'-1,m}) = 2^{n-d-g'+k'-1}\sigma(T_1) + \sigma(T_1'). \tag{2.4}$$

Furthermore,

$$\begin{aligned}
\sigma(T_1) &= \sigma(T_1-u_{1'}) + \sigma(T_1-N[u_{1'}])\\
&= \sigma(P_{m-1}\cup P_{x-2}\cup T_2) + \sigma(P_{m-2}\cup P_{x-3}\cup T_2')\\
&= F_mF_{x-1}\sigma(T_2) + F_{m-1}F_{x-2}\sigma(T_2')\\
&= F_mF_{x-1}[\sigma(T_2-u_{k'}) + \sigma(T_2-N[u_{k'}])] + F_{m-1}F_{x-2}[\sigma(T_2'-u_{k'}) + \sigma(T_2'-N[u_{k'}])]\\
&= F_mF_{x-1}[\sigma(P_{y-2}\cup P_l\cup P_{k'-2}) + \sigma(P_{y-3}\cup P_{l-1}\cup P_{k'-3})] + F_{m-1}F_{x-2}[\sigma(P_{y-2}\cup P_l\cup P_{k'-3})\\
&\quad + \sigma(P_{y-3}\cup P_{l-1}\cup P_{k'-4})]\\
&= F_mF_{x-1}F_{y-1}F_{l+1}F_{k'-1} + F_mF_{x-1}F_{y-2}F_lF_{k'-2} + F_{m-1}F_{x-2}F_{y-1}F_{l+1}F_{k'-2} + F_{m-1}F_{x-2}F_{y-2}F_lF_{k'-3}.
\end{aligned} \tag{2.5}$$

Similarly,

$$\sigma(T_1') = F_mF_{x-2}F_{y-2}F_{l+1}F_{k'-1} + F_mF_{x-2}F_{y-3}F_lF_{k'-2} + F_{m-1}F_{x-3}F_{y-2}F_{l+1}F_{k'-2} + F_{m-1}F_{x-3}F_{y-3}F_lF_{k'-3}. \tag{2.6}$$

From (2.4)–(2.6) we get

$$\begin{aligned}\sigma(\bar{U}^{g',h'}_{n+k-d-g'-1,m}) = {} & (2^{n-d-g'+k'-1}-1)(F_mF_{x-1}F_{y-1}F_{l+1}F_{k'-1}+F_mF_{x-1}F_{y-2}F_lF_{k'-2}\\ & +F_{m-1}F_{x-2}F_{y-1}F_{l+1}F_{k'-2}+F_{m-1}F_{x-2}F_{y-2}F_lF_{k'-3})+F_mF_{g'-k'+1}F_{l+1}F_{k'-1}\\ & +F_mF_{g'-k'}F_lF_{k'-2}+F_{m-1}F_{g'-k'}F_{l+1}F_{k'-2}+F_{m-1}F_{g'-k'-1}F_lF_{k'-3}.\end{aligned}$$

Similarly, we can show that (iii), (iv) are, respectively, true.

This completes the proof of Lemma 2.2. □

Lemma 2.3. *For positive integers g', k', if $g'-k' \geqslant 2$, then*

(i) $\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) \geq \sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m})$;
(ii) $\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) \geq \sigma(\bar{U}^{g',h'}_{n+k'-d-g'-1,m})$;
(iii) $\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) \geq \sigma(\bar{U}^{g',t'}_{n+k'-d-g'-1,m})$;
(iv) $\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) \geq \sigma(\bar{U}^{g',j}_{n+k'-d-g'-1,m})$.

Proof. Note that in $U^{g'}_d$, $l = d-m-k'+2$.

(i) By Lemmas 2.1 and 2.2,

$$\begin{aligned}&\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1})-\sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m})\\ &= 2^{n-d-g'+k'-1}F_{m+k'-1}F_{l+1}F_{g'-k'+1}+F_{m+k'-2}F_lF_{g'-k'-1}-\sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m})\\ &= 2^{n-d-g'+k'-1}[F_{l+1}(F_mF_{k'-1}+F_{m-1}F_{k'-2})F_{g'-k'+1}-F_{l+1}F_mF_{g'-k'+1}F_{k'-1}\\ &\quad -F_{l+1}F_{m-1}F_{g'-k'}F_{k'-2}]+F_lF_mF_{k'-2}F_{g'-k'-1}+F_lF_{m-1}F_{k'-3}F_{g'-k'-1}- F_lF_{g'-k'}(F_mF_{k'-2}-F_{m-1}F_{k'-3})\\ &= 2^{n-d-g'+k'-1}(F_{l+1}F_{g'-k'+1}F_{m-1}F_{k'-2}-F_{l+1}F_{m-1}F_{g'-k'}F_{k'-2})+F_lF_mF_{k'-2}F_{g'-k'-1}\\ &\quad +F_lF_{m-1}F_{k'-3}F_{g'-k'-1}-F_lF_mF_{k'-2}F_{g'-k'}-F_lF_{m-1}F_{k'-3}F_{g'-k'-1}\\ &= 2^{n-d-g'+k'-1}F_{l+1}F_{m-1}F_{k'-2}F_{g'-k'-1}-F_lF_mF_{k'-2}F_{g'-k'-2}\\ &\geqslant 2(F_l+F_{l-1})F_{m-1}F_{k'-2}(F_{g'-k'-2}+F_{g'-k'-3})-F_l(F_{m-1}+F_{m-2})F_{k'-2}F_{g'-k'-2}\\ &\geqslant F_{l-1}F_{m-1}F_{g'-k'-2}F_{k'-2}>0.\end{aligned}$$

Therefore,

$$\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) > \sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1,m}).$$

(iii) Note that in $U^{g'}_d$, $k' = x'+y'-1$, by Lemmas 2.1 and 2.2,

$$\begin{aligned}&\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1})-\sigma(\bar{U}^{g',t'}_{n+k'-d-g'-1,m})\\ &\geqslant F_mF_{l+1}F_{x'-2}F_{y'-2}F_{g'-k'+1}+F_{m-1}F_{l+1}F_{x'-1}F_{y'-2}F_{g'-k'+1}+F_{m-1}F_{l+1}F_{x'-2}F_{y'-3}F_{g'-k'+1}\\ &\quad +F_mF_lF_{x'-1}F_{y'-2}F_{g'-k'-1}+F_mF_lF_{x'-2}F_{y'-3}F_{g'-k'-1}+F_{m-1}F_lF_{x'-3}F_{y'-3}F_{g'-k'-1}\\ &\quad -F_mF_lF_{x'-1}F_{y'-2}F_{g'-k'}-F_{m-1}F_{l+1}F_{x'-2}F_{y'-1}F_{g'-k'}+F_{m-1}F_{l+1}F_{x'-2}F_{y'-2}F_{g'-k'-1}\\ &\quad +F_{m-1}F_{l+1}F_{x'-3}F_{y'-2}F_{g'-k'-1}-F_mF_lF_{x'-1}F_{y'-2}F_{g'-k'-2}-F_mF_lF_{x'-2}F_{y'-3}F_{g'-k'-2}\\ &= F_mF_lF_{x'-4}F_{y'-2}F_{g'-k'-1}+F_mF_{l-1}F_{x'-2}F_{y'-2}F_{g'-k'+1}+F_{m-1}F_{l+1}F_{x'-3}F_{y'-2}F_{g'-k'+1}\\ &\quad +F_mF_lF_{x'-2}F_{y'-1}F_{g'-k'-3}+F_{m-1}F_lF_{x'-3}F_{y'-3}F_{g'-k'-1}-F_mF_lF_{x'-3}F_{y'-2}F_{g'-k'-4}\\ &\quad +F_{m-1}F_{l+1}F_{x'-3}F_{y'-2}F_{g'-k'-1}+F_{m-1}F_{l+1}F_{x'-2}F_{y'-1}(F_{g'-k'+1}-F_{g'-k'-2})\\ &> F_{m-1}F_{l+1}F_{x'-2}F_{y'-1}(F_{g'-k'+1}-F_{g'-k'-2})>0.\end{aligned}$$

Therefore,

$$\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) > \sigma(\bar{U}^{g',t'}_{n+k'-d-g'-1,m}).$$

Similarly, we can show that (ii) and (iv) hold.

Lemma 2.4. $\sigma(U^{g-k,j}_{n+k-d-g}) > \sigma(U^{g-k+1,j}_{n+k-d-g-1})$ *for $g-k \geqslant 3$.*

Proof. By Lemma 2.1, we have

$$\begin{aligned}
&\sigma(U^{g-k,j}_{n+k-d-g}) - \sigma(U^{g-k+1,j}_{n+k-d-g-1})\\
&\quad = 2^{n-d-g+k-1}(2F_jF_{d+2-j}F_{g-k} - F_jF_{d+2-j}F_{g-k+1}) + F_{j-1}F_{d+1-j}F_{g-k-2} - F_{j-1}F_{d+1-j}F_{g-k-1}\\
&\quad \geq F_jF_{d+2-j}(2F_{g-k} - F_{g-k+1}) + F_{j-1}F_{d+1-j}(F_{g-k-2} - F_{g-k-1})\\
&\quad = F_jF_{d+2-j}F_{g-k-2} - F_{j-1}F_{d+1-j}F_{g-k-3} > 0.
\end{aligned}$$

Hence, we have $\sigma(U^{g-k,j}_{n+k-d-g}) > \sigma(U^{g-k+1,j}_{n+k-d-g-1})$. $\square$

Corollary 2.5. $\sigma(U^{3,j}_{n-d-3}) > \sigma(U^{4,j}_{n-d-4}) > \cdots > \sigma(U^{n-d,j}_{0})$.

Lemma 2.6. *Let $d+2 = 4s+r$, where n, s and r are integers with $0 \leqslant r \leqslant 3$.*

(i) *For $r \in \{0, 1\}$, we have*

$$\sigma(U^{g-k+1,2}_{n-d-g+k-1}) > \sigma(U^{g-k+1,4}_{n-d-g+k-1}) > \cdots > \sigma(U^{g-k+1,2s}_{n-d-g+k-1}) > \sigma(U^{g-k+1,2s-1}_{n-d-g+k-1}) > \cdots > \sigma(U^{g-k+1,1}_{n-d-g+k-1}); \tag{2.7}$$

(ii) *For $r \in \{2, 3\}$, we have*

$$\begin{aligned}
&\sigma(U^{g-k+1,2}_{n-d-g+k-1}) > \sigma(U^{g-k+1,4}_{n-d-g+k-1}) > \cdots > \sigma(U^{g-k+1,2s}_{n-d-g+k-1}) > \sigma(U^{g-k+1,2s+1}_{n-d-g+k-1})\\
&\quad > \sigma(U^{g-k+1,2s-1}_{n-d-g+k-1}) > \cdots > \sigma(U^{g-k+1,1}_{n-d-g+k-1}).
\end{aligned} \tag{2.8}$$

Proof. By Lemma 2.1,

$$\begin{aligned}
\sigma(U^{g-k+1,j}_{n-d-g+k-1}) &= 2^{n-d-g+k-1}F_jF_{d+2-j}F_{g-k+1} + F_{j-1}F_{d+1-j}F_{g-k-1}\\
&= (2^{n-d-g+k-1}F_{g-k+1} - F_{g-k-1})F_jF_{d+2-j} + F_{g-k-1}F_{d+2}.
\end{aligned}$$

(i) For $r \in \{0, 1\}$, by Lemma 1.2 (i),

$$F_2F_d > F_4F_{d-2} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} > \cdots > F_1F_{d+1}$$

and the inequality in (2.7) follows from this.

(ii) For $r \in \{2, 3\}$, by Lemma 1.2 (ii),

$$F_2F_d > F_4F_{d-2} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} > F_{2s-1}F_{2s+r+1} > \cdots > F_1F_{d+1}$$

and the inequality in (2.8) follows from this.

This completes the proof of Lemma 2.6. $\square$

In view of Lemma 2.6, the following corollary is obvious.

Corollary 2.7. $\sigma(U^{3,2}_{n-d-3}) > \sigma(U^{3,4}_{n-d-3}) > \cdots > \sigma(U^{3,2s}_{n-d-3}) > \sigma(U^{3,2s-1}_{n-d-3}) > \cdots > \sigma(U^{3,3}_{n-d-3})$.

Let $\mathcal{U}_{n,d} = \mathcal{U}^1_{n,d} \bigcup \mathcal{U}^2_{n,d}$, where $\mathcal{U}^1_{n,d} = \{U : U \in \mathcal{U}_{n,d}$, there exist $C_{g'}$ and P_{d+1} in U such that $g' - |V(C_{g'}) \cap V(P_{d+1})| \geqslant 2\}$, $\mathcal{U}^2_{n,d} = \{U : U \in \mathcal{U}_{n,d}$, there exist $C_{g'}$ and P_{d+1} in U such that $g' - |V(C_{g'}) \cap V(P_{d+1})| = 1\}$.

Theorem 2.8. *If $G \in \mathcal{U}^1_{n,d}$, then $\sigma(G) \leqslant 6 \cdot 2^{n-d-3}F_d + F_{d-1}$, the equality holds if, and only if, $G \cong U^{3,2}_{n-d-3}$.*

Proof. By Lemma 2.1, we have

$$\sigma(U^{3,2}_{n-d-3}) = 6 \cdot 2^{n-d-3}F_d + F_{d-1}. \tag{2.9}$$

Let $G \in \mathcal{U}_{n,d}$ and let P be a path of length d in G.

Case 1. $P \cap C_{g'} \neq \emptyset$. Without loss of generality, we assume that P and $C_{g'}$ possess exactly k vertices in common. Then the arrangement of P and $C_{g'}$ in G is the same as in $U^{g'}_d$ in Fig. 1.

Set $V^*(G) := \{u : u \in V(U^{g'}_d) \setminus \{u_{1'}, u_{k'}\}$ and $d(u) \geqslant 3\} \cup \{u_{1'} : d(u_{1'}) \geqslant 4\} \cup \{u_{k'} : d(u_{k'}) \geqslant 4\}$, assume $|V^*(G)| = m$, then relabel the vertices in $V^*(G)$ as $x_1, x_2, \ldots, x_m$. For each $x_i \in V^*(G)$, $i = 1, \ldots, m$, let T_i be a subtree of $G - E(U^{g'}_d)$ which contains x_i and $|V(T_i)| = p_i + 1$. Denote

$$H = U^{g'}_d \cup \left(\bigcup_{1 \leqslant j \leqslant m, j \neq i} T_j \right),$$

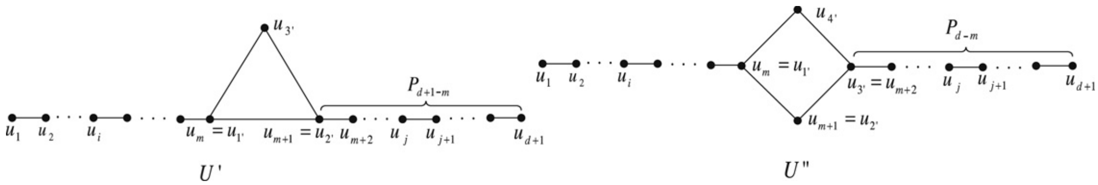

Fig. 4. Graphs U' and U''.

then $G = Hx_iT_i$. By Lemma 1.4, we have $\sigma(Hx_iT_i) \leqslant \sigma(Hx_iK_{1,p_i})$. Thus repeated using Lemma 1.4,

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, p_2, \dots, p_i, \dots, p_m)),$$

where $U_d^{g'}(p_1, p_2, \dots, p_i, \dots, p_m)$ is a unicyclic graph of order n with diameter d created from $U_d^{g'}$ by attaching p_i pendent vertices to $x_i \in V^*(G)$, $1 \leqslant i \leqslant m$, respectively. Corresponding to $x_i, x_j \in V^*(G)$, let

$$X = K_{1,p_i}, \quad Y = K_{1,p_j}, \quad \text{and} \quad H' = G - VL(K_{1,p_i}) - VL(K_{1,p_j}),$$

then $U_d^{g'}(p_1, p_2, \dots, p_m) = Xx_iH'x_jY$. By Lemma 1.3, we have either

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \sigma(U_d^{g}(p_1, \dots, p_i + p_j, \dots, 0, \dots, p_m)),$$

or

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \sigma(U_d^{g}(p_1, \dots, 0, \dots, p_i + p_j, \dots, p_m)).$$

Repeated using above step, we obtain either

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \cdots < \sigma(\bar{U}^{g',k'}_{n+k'-d-g'-1}), \tag{2.10}$$

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \cdots < \sigma(\bar{U}^{g',h'}_{n+k'-d-g'-1}), \tag{2.11}$$

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \cdots < \sigma(\bar{U}^{g',t'}_{n+k'-d-g'-1}), \tag{2.12}$$

or

$$\sigma(G) \leqslant \sigma(U_d^{g'}(p_1, \dots, p_i, \dots, p_j, \dots, p_m)) < \cdots < \sigma(\bar{U}^{g',j}_{n+k'-d-g'-1}). \tag{2.13}$$

Together with (2.10)–(2.13) and Lemma 2.3, we obtain that

$$\sigma(G) < \sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}).$$

By Corollaries 2.5 and 2.7,

$$\sigma(U^{g'-k'+1,m+k'-1}_{n-d-g'+k'-1}) < \sigma(U^{3,m+k'-1}_{n-d-3}) < \sigma(U^{3,2}_{n-d-3}).$$

Therefore, $\sigma(G) < \sigma(U^{3,2}_{n-d-3}) = 6 \cdot 2^{n-d-3}F_d + F_{d-1}$.

Case 2. $P \cap C_{g'} = \emptyset$. Then cycle $C_{g'}$ connects to P by a path of length at least 1. By Lemma 1.3, we can obtain a unicyclic graph $G' \in U_d^{g'}$ such that $\sigma(G) < \sigma(G')$ and the cycle $C_{g'}$ and P in G' possess exactly one vertex in common. By Case 1, $\sigma(G) < \sigma(G') \leqslant 6 \cdot 2^{n-d-3}F_d + F_{d-1}$.

By Cases 1 and 2, we obtain that if $G \in \mathcal{U}^1_{n,d}$, then $\sigma(G) \leqslant 6 \cdot 2^{n-d-3}F_d + F_{d-1}$, the equality holds if and only if $G \cong U^{3,2}_{n-d-3}$. $\square$

In the following we shall determine the graph G in $\mathcal{U}^2_{n,d}$ with the maximum Fibonacci number. It is straightforward to check that, in this case, the length of the cycle in G is either 3 or 4. The arrangement of the longest path and the cycle contained in G is as U' or U''; see Fig. 4.

By definition, $\bar{U}^{3,i}_{n-d-2,m}$ (respectively, $\bar{U}^{3,1'}_{n-d-2,m}, \bar{U}^{3,2'}_{n-d-2,m}, \bar{U}^{3,3'}_{n-d-2,m}, \bar{U}^{3,j}_{n-d-2,m}$) is the unicyclic graph with diameter d created from U' by attaching $n-d-2$ pendent vertices to the vertex u_i (respectively, $u_{1'}, u_{2'}, u_{3'}, u_j$). Similarly, $\bar{U}^{4,i}_{n-d-2,m}$ (respectively, $\bar{U}^{4,1'}_{n-d-2,m}, \bar{U}^{4,3'}_{n-d-2,m}, \bar{U}^{4,4'}_{n-d-2,m}, \bar{U}^{4,j}_{n-d-2,m}$) is the unicyclic graph with diameter d created from U'' by attaching $n-d-2$ pendent vertices to the vertex u_m (respectively, $u_i, u_{3'}, u_{4'}, u_j$).

Lemma 2.9. *For a fixed positive integer m, we have*

(i) $\sigma(\bar{U}^{3,1'}_{n-d-2,m}) > \sigma(\bar{U}^{3,3'}_{n-d-2,m})$ *and* $\sigma(\bar{U}^{3,1'}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{3,i}_{n-d-2,m})$ *for* $1 \leqslant i \leqslant m$*, the equality holds if, and only if,* $i = m$.

(ii) $\sigma(\bar{U}^{3,2'}_{n-d-2,m}) > \sigma(\bar{U}^{3,3'}_{n-d-2,m})$ *and* $\sigma(\bar{U}^{3,2'}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{3,j}_{n-d-2,m})$ *for* $m+1 \leqslant j < d+1$*, the equality holds if, and only if,* $j = m+1$.

Proof. Set $l = d + 1 - m$, by Lemma 1.1 we have

$$\sigma(\bar{U}^{3,1'}_{n-d-2,m}) = (2^{n-d-2} - 1)F_mF_{d+3-m} + F_mF_{d+1-m} + F_{d+2}, \tag{2.14}$$

$$\sigma(\bar{U}^{3,2'}_{n-d-2,m}) = (2^{n-d-2} - 1)F_{m+2}F_{d+1-m} + F_mF_{d+1-m} + F_{d+2}, \tag{2.15}$$

$$\sigma(\bar{U}^{3,i}_{n-d-2,m}) = (2^{n-d-2} - 1)F_i(F_{d+2-i}F_l + F_{m-i}F_{d+1-m}) + F_mF_{d+1-m} + F_{d+2},$$

$$\sigma(\bar{U}^{3,j}_{n-d-2,m}) = (2^{n-d-2} - 1)F_{d+2-j}(F_{m+2}F_{j-m-1} + F_mF_{j-m-2}) + F_mF_{d+1-m} + F_{d+2},$$

$$\sigma(\bar{U}^{3,3'}_{n-d-2,m}) = 2^{n-d-2}F_{d+2} + F_mF_{d+1-m} + F_{d+2}.$$

(i)

$$\sigma(\bar{U}^{3,1'}_{n-d-2,m}) - \sigma(\bar{U}^{3,3'}_{n-d-2,m}) = (2^{n-d-2} - 1)F_{m-2}F_{d+1-m}.$$

Note that $d + 1 > m$ and $m \geqslant 2$ (otherwise, the diameter of $\bar{U}^{3,m}_{n-d-2,m}$ is $d + 1$, a contradiction), therefore, $(2^{n-d-2} - 1)F_{m-2}F_{d+1-m} > 0$, i.e., $\sigma(\bar{U}^{3,m}_{n-d-2,m}) > \sigma(\bar{U}^{3,3'}_{n-d-2,m})$.

$$\sigma(\bar{U}^{3,1'}_{n-d-2,m}) - \sigma(\bar{U}^{3,i}_{n-d-2,m}) = (2^{n-d-2} - 1)F_{m-i-1}(F_{i-1}F_{d+2-m} - F_{i-2}F_{d+1-m}). \tag{2.16}$$

Note that $i \geqslant 2$ (otherwise, the diameter of $\bar{U}^{3,i}_{n-d-2,m}$ is $d + 1$, a contradiction) and $d + 2 - m > 0$, thus $F_{i-1}F_{d+2-m} - F_{i-2}F_{d+1-m} > 0$. On the other hand, $F_{m-i-1} \geqslant 0$, the equality holds if, and only if, $m = i$. By (2.16) we obtain $\sigma(\bar{U}^{3,m}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{3,i}_{n-d-2,m})$, and the equality holds if, and only if, $m = i$.

(ii)

$$\sigma(\bar{U}^{3,2'}_{n-d-2,m}) - \sigma(\bar{U}^{3,3'}_{n-d-2,m}) = (2^{n-d-2} - 1)F_mF_{d-1-m} > 0.$$

Therefore, $\sigma(\bar{U}^{3,2'}_{n-d-2,m}) > \sigma(\bar{U}^{3,3'}_{n-d-2,m})$.

$$\sigma(\bar{U}^{3,2'}_{n-d-2,m}) - \sigma(\bar{U}^{3,j}_{n-d-2,m}) = (2^{n-d-2} - 1)F_{j-m-2}(F_{m+1}F_{d+1-j} - F_mF_{d-j}).$$

Note that $F_{m+1}F_{d+1-j} - F_mF_{d-j} > 0$ and $F_{j-m-2} \geqslant 0$, the equality holds if, and only if, $j = m + 1$, thus $\sigma(\bar{U}^{3,2'}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{3,j}_{n-d-2,m})$, and equality holds if, and only if, $j = m + 1$. $\square$

Corollary 2.10. *$\bar{U}^{3,1'}_{n-d-2,2}$ is the graph with the maximum Fibonacci number in $\{\bar{U}^{3,1'}_{n-d-2,m} : 2 \leqslant m \leqslant d - 2\} \bigcup \{\bar{U}^{3,2'}_{n-d-2,m} : 2 \leqslant m \leqslant d - 2\}$.*

Proof. By Lemma 1.2 and Eqs. (2.14) and (2.15), we know that $\bar{U}^{3,1'}_{n-d-2,2}$ is the graph with the maximum Fibonacci number in $\{\bar{U}^{3,1'}_{n-d-2,m} : 2 \leq m \leqslant d - 2\}$ and $\bar{U}^{3,2'}_{n-d-2,2}$ is the graph with the maximum Fibonacci number in $\{\bar{U}^{3,2'}_{n-d-2,m} : 2 \leq m \leqslant d - 2\}$. On the other hand,

$$\bar{U}^{3,2'}_{n-d-2,2} - \bar{U}^{3,1'}_{n-d-2,2} = (2^{n-d-2} - 1)(F_{d-3} - F_{d-2}) \leqslant 0,$$

the equality holds if, and only if, $d = 3$. It is easy to see when $d = 3$, $\bar{U}^{3,2'}_{n-5,2} = \bar{U}^{3,1'}_{n-5,2}$. This completes the proof. $\square$

Lemma 2.11. *For a fixed positive integer m, we have*

(i) $\sigma(\bar{U}^{4,1'}_{n-d-2,m}) > \sigma(\bar{U}^{4,4'}_{n-d-2,m})$ *and* $\sigma(\bar{U}^{4,1'}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{4,i}_{n-d-2,m})$ *for* $1 < i \leq m$*, the equality holds if, and only if,* $i = m$.

(ii) $\sigma(\bar{U}^{4,3'}_{n-d-2,m}) > \sigma(\bar{U}^{4,4'}_{n-d-2,m})$ *and* $\sigma(\bar{U}^{4,3'}_{n-d-2,m}) \geqslant \sigma(\bar{U}^{4,j}_{n-d-2,m})$ *for* $m + 2 \leq j < d + 1$*, the equality holds if, and only if,* $j = m + 2$.

Corollary 2.12. *$\bar{U}^{4,1'}_{n-d-2,2}$ is the graph with the maximum Fibonacci number in $\{\bar{U}^{4,1'}_{n-d-2,m} : 2 \leqslant m \leqslant d - 2\} \bigcup \{\bar{U}^{4,3'}_{n-d-2,m} : 2 \leqslant m \leqslant d - 3\}$.*

Lemma 2.11 and Corollary 2.12 can be proved in the same way as Lemma 2.9 and Corollary 2.10, respectively. We will not repeat the procedure here.

Summarizing Corollaries 2.10 and 2.12, we arrived at:

Theorem 2.13. *Let $G \in \mathcal{U}^2_{n,d}$.*

(i) *If* $d \geqslant 4$*, then* $\sigma(G) \leq 2^{n-d-1}(2F_{d-2} + F_d) + F_{d-1}$*, the equality holds if, and only if,* $G \cong \bar{U}^{4,1'}_{n-d-2,2}$.

(ii) *If* $d = 3$*, then* $\bar{U}^{3,1'}_{n-5,2}$ *is the unique graph with maximum Fibonacci number in* $\mathcal{U}^2_{n,d}$

Note that when $d \geqslant 4$,

$$\sigma(\bar{U}^{4,1'}_{n-d-2,2}) = 2^{n-d-1}(2F_{d-2} + F_d) + F_{d-1}. \tag{2.17}$$

By Eqs. (2.9) and (2.17), it is easy to see that

$$\sigma(\bar{U}^{4,1'}_{n-d-2,2}) > \sigma(U^{3,2}_{n-d-3}). \tag{2.18}$$

When $d = 3$, by (2.8) and (2.13), we have

$$\sigma(\bar{U}^{3,1'}_{n-5,2}) > \sigma(U^{3,2}_{n-6}). \tag{2.19}$$

Summarizing Theorems 2.8 and 2.13 and (2.18)–(2.19), we obtain the main results of this paper.

Theorem 2.14. *Let $G \in \mathcal{U}_{n,d}$.*

(i) *If $d = 3$, then $\sigma(G) \leqslant 5 \cdot 2^{n-4} + 2$, the equality holds if, and only if, $G \cong \bar{U}^{3,1'}_{n-5,2}$.*

(ii) *If $d \geqslant 4$, then $\sigma(G) \leqslant 2^{n-d-1}(2F_{d-2} + F_d) + F_{d-1}$, the equality holds if, and only if, $G \cong \bar{U}^{4,1'}_{n-d-2}$.*

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